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Vivek Shenoy, Brian Sheldon

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14. ABSTRACT
This report describes the progress made as part of the subject contract. The work resulted in 17 papers, over 25 invited talks and training of two postdoctoral candidates, one graduate student. The theoretical work on thermal, electronic and optical properties of 2D materials led to several new experimentalists to validate our predictions.

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2D materials, multi scale modeling

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a. REPORT	b. ABSTRACT	c. THIS PAGE			Brian Sheldon
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Report Title

Multi-scale modeling, design strategies and physical properties of 2D composite sheets: Final Report

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This report describes the progress made as part of the subject contract. The work resulted in 17 papers, over 25 invited talks and training of two postdoctoral candidates, one graduate student. The theoretical work on thermal, electronic and optical properties of 2D materials led to several new experimentalists to validate our predictions.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received		Paper
08/27/2012	4.00	Vivek B. Shenoy, Yu Xiao, Kaushik Bhattacharya. Effect of doping on polarization profiles and switching in semiconducting ferroelectric thin films, Journal of Applied Physics, (2012): 0. doi: 10.1063/1.3702849
08/27/2012	7.00	Vivek Shenoy, David Gracias. Self-folding thin-film materials: From nanopolyhedra to graphene origami, MRS Bulletin, (10 2012): 0. doi:
08/27/2012	6.00	Vivek B. Shenoy, Priya Johari. Tuning the Electronic Properties of Semiconducting Transition Metal Dichalcogenides by Applying Mechanical Strains, ACS Nano, (06 2012): 0. doi: 10.1021/nn301320r
08/27/2012	3.00	Pekka Koskinen, Oleg O. Kit, Vivek B. Shenoy, Ashwin Ramasubramaniam. Edge-stress-induced spontaneous twisting of graphene nanoribbons, Journal of Applied Physics, (2012): 0. doi: 10.1063/1.3689814
08/27/2012	5.00	Priya Johari, Vivek B. Shenoy. Modulating Optical Properties of Graphene Oxide: Role of Prominent Functional Groups, ACS Nano, (09 2011): 0. doi: 10.1021/nn202732t
09/22/2014	8.00	Dequan Er, Junwen Li, Michael Naguib, Yury Gogotsi, Vivek B. Shenoy. Ti?C? MXene as a high capacity electrode material for metal (Li, Na, K, Ca) ion batteries, ACS Applied Materials & Interfaces, (07 2014): 0. doi: 10.1021/am501144q
09/22/2014	9.00	Dibakar Datta, Junwen Li, Nikhil Koratker, Vivek B. Shenoy. Enhanced lithiation in defective graphene, Carbon, (08 2014): 0. doi: 10.1016/j.carbon.2014.08.068
09/22/2014	10.00	Rahul Mukherjee, Abhay V. Thomas, Dibakar Datta, Eklavya Singh, Junwen Li, Osman Eksik, Vivek B. Shenoy, Nikhil Koratkar. Defect-induced plating of lithium metal within porous graphene networks, Nature Communications, (04 2014): 0. doi: 10.1038/ncomms4710
09/22/2014	11.00	Sina Najmaei, Xiaolong Zou, Dequan Er, Junwen Li, Zehua Jin, Weilu Gao, Qi Zhang, Sooyoun Park, Liehui Ge, Sidong Lei, Junichiro Kono, Vivek B. Shenoy, Antony George, Pulickel M. Ajayan, Jun Lou. Tailoring the Physical Properties of Molybdenum Disulfide Monolayers by Control of Interfacial Chemistry, Nano Letters, (03 2014): 0. doi: 10.1021/nl404396p
09/22/2014	12.00	Dibakar Datta, Junwen Li, Vivek B. Shenoy. Defective Graphene as a High-Capacity Anode Material for Na- and Ca-Ion Batteries, ACS Applied Materials & Interfaces, (02 2014): 0. doi: 10.1021/am404788e
09/22/2014	13.00	Damien Voiry, Maryam Salehi, Rafael Silva, Takeshi Fujita, Mingwei Chen, Tewodros Asefa, Vivek B. Shenoy, Goki Eda, Manish Chhowalla. Conducting MoS2 Nanosheets as Catalysts for Hydrogen Evolution Reaction, Nano Letters, (12 2013): 0. doi: 10.1021/nl403661s
09/22/2014	14.00	Esteban Meca, John Lowengrub, Hokwon Kim, Cecilia Mattevi, Vivek B. Shenoy. Epitaxial Graphene Growth and Shape Dynamics on Copper: Phase-Field Modeling and Experiments, Nano Letters, (11 2013): 0. doi: 10.1021/nl4033928

09/22/2014 15.00 Qing-Xiang Pei, Yong-Wei Zhang, Zhen-Dong Sha, Vivek B. Shenoy. Tuning the thermal conductivity of silicene with tensile strain and isotopic doping: A molecular dynamics study, Journal of Applied Physics, (2013): 0. doi: 10.1063/1.4815960

09/22/2014 16.00 Nikhil V. Medhekar, Vivek B. Shenoy, Junwen Li. Bonding Charge Density and Ultimate Strength of Monolayer Transition Metal Dichalcogenides, The Journal of Physical Chemistry C, (08 2013): 0. doi: 10.1021/jp403986v

09/22/2014 17.00 Damien Voiry, Hisato Yamaguchi, Junwen Li, Rafael Silva, Diego C. B. Alves, Takeshi Fujita, Mingwei Chen, Tewodros Asefa, Vivek B. Shenoy, Goki Eda, Manish Chhowalla. Enhanced catalytic activity in strained chemically exfoliated WS2 nanosheets for hydrogen evolution, Nature Materials, (07 2013): 0. doi: 10.1038/nmat3700

09/26/2011 1.00 Priya Johari, Vivek B. Shenoy. Tunable Dielectric Properties of Transition Metal Dichalcogenides, ACS Nano, (07 2011): 0. doi: 10.1021/nn201698t

09/26/2011 2.00 Akbar Bagri, Sang-Pil Kim, Rodney S. Ruoff, Vivek B. Shenoy. Thermal transport across Twin Grain Boundaries in Polycrystalline Graphene from Nonequilibrium Molecular Dynamics Simulations, Nano Letters, (09 2011): 0. doi: 10.1021/nl202118d

TOTAL: **17**

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received Paper

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received Paper

TOTAL:

Number of Manuscripts:

Books

Received Book

TOTAL:

Received Book Chapter

TOTAL:

Patents Submitted

Patents Awarded

Awards

Graduate Students

NAME	PERCENT SUPPORTED	Discipline
Dibakar Datta	1.00	
FTE Equivalent:	**1.00**	
Total Number:	**1**	

Names of Post Doctorates

NAME	PERCENT SUPPORTED
Junwen Li	1.00
FTE Equivalent:	**1.00**
Total Number:	**1**

Names of Faculty Supported

NAME	PERCENT SUPPORTED	National Academy Member
Vivek Shenoy	0.20	
Brian Sheldon	0.01	
FTE Equivalent:	**0.21**	
Total Number:	**2**	

Names of Under Graduate students supported

NAME	PERCENT SUPPORTED	Discipline
Clark Shurtleff?	0.00	Materials Science
Kevin Zhai	0.00	Materials Science
FTE Equivalent:	**0.00**	
Total Number:	**2**	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 2.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:..... 2.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:..... 1.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):..... 2.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields: 0.00

Names of Personnel receiving masters degrees

NAME
Total Number:

Names of personnel receiving PHDs

NAME
Dibakar Datta
Total Number: 1

Names of other research staff

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

We made progress in the following areas: 1) Predicting the influence of defects on thermal transport through 2D crystalline materials, 2) Predicting the optical properties of 2D materials and 3) prediction of methods to engineer the electronic properties of 2D materials through strain engineering, 4) Prediction and experimental validation of how defects can increase the storage capacity of Lithium in 2D materials and 5) Development of a new multiscale method to predict the growth of 2D materials. Our work led to 17 publications and ~35 invited/plenary talks at major conferences (MRS, ACS, APS, ASME, SES), national labs (Oak Ridge, Ames, Los Alamos, ARL), and national and international universities. We also initiated collaboration with other ARO PIs and ARL labs. Our work has led to new experimental work on thermal transport, strain engineering, energy storage and growth.

Technology Transfer